John von Neumann Institute for Computing

# Hadron Spectrum of QCD with one Quark Flavour

F. Farchioni, I. Montvay, G. Münster, E. E. Scholz,
T. Sudmann, J. Wuilloud

published in

*NIC Symposium 2008*,
G. Münster, D. Wolf, M. Kremer (Editors),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **39**, ISBN 978-3-9810843-5-1, pp. 127-134, 2008.



http://www.fz-juelich.de/nic-series/volume39

# Hadron Spectrum of QCD with one Quark Flavour

**Federico Farchioni**[1], **István Montvay**[2], **Gernot Münster**[1], **Enno E. Scholz**[3], **Tobias Sudmann**[1], **and Jaïr Wuilloud**[1]

[1] Universität Münster, Institut für Theoretische Physik
Wilhelm-Klemm-Strasse 9, D-48149 Münster, Germany
*E-mail: munsteg@uni-muenster.de*

[2] Deutsches Elektronen-Synchrotron DESY
Notkestr. 85, D-22603 Hamburg, Germany

[3] Physics Department, Brookhaven National Laboratory
Upton, NY 11973, USA

The hadron spectrum of Quantum Chromodynamics with a single flavour of quarks is studied by Monte Carlo simulations at two different lattice spacings. The lightest simulated quark mass corresponds to a pion with mass $\sim 270$ MeV. The symmetry of the single flavour theory can be artificially enhanced by adding extra valence quarks, which can be interpreted as $u$ and $d$ quarks. Properties of the theory are analyzed by making use of the ideas of partially quenched chiral perturbation theory applied to the extended theory.

## 1 Introduction and Motivation

For the strong interactions of elementary particles a successful theoretical description exists in terms of Quantum Chromodynamics (QCD). In the low-energy regime of QCD perturbation theory ceases to be applicable. In particular, to calculate the spectrum of physical particles from QCD is a genuine non-perturbative problem. This is where numerical simulations of QCD by means of the Monte Carlo method turn out to be an indispensable and very powerful tool.

To include the dynamics of quarks in numerical simulations is an important but demanding task. It requires the calculation of the determinant of the quadratic form describing fermions in the QCD action, and consumes most of the computer time. Due to the development of computer power, it has become possible in recent years to include the dynamics of quarks in QCD simulations.

Quarks do not exist as isolated particles, but bind together in mesons and baryons. Therefore it is not possible to give a straightforward unique definition of quark masses. In recent years M. Creutz has drawn the attention to open problems in QCD, which show up in this context[1,2]. One question raised by Creutz, having a relevant phenomenological impact, is whether it is possible to define in an unambiguous way the case where *one* quark (say the $u$ quark) becomes massless. The arguments against an unique definition of the massless limit[1] especially hold for the one-flavour theory.

A difference between QCD with more than one quark flavour ($N_f > 1$) and QCD with a single flavour ($N_f = 1$), which plays a crucial role in this context, is the nature of chiral symmetry. The Lagrangian of QCD with $N_f > 1$ flavours of massless quarks possesses a continuous chiral symmetry with symmetry group $\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R \otimes \mathrm{U}(1)_A$. In the quantum theory the axial $\mathrm{U}(1)_A$ is not a symmetry due to the Adler-Bell-Jackiw anomaly.

The remaining $\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R$ chiral symmetry is broken spontaneously to its diagonal subgroup, which is the usual $\mathrm{SU}(N_f)$ vector symmetry. The Goldstone bosons associated with the spontaneous symmetry breakdown are massless pseudoscalar mesons, e.g. the pions and kaons. If quark masses $m_q$ are turned on, the Goldstone bosons acquire masses. If the quark masses are equal and small, the masses of the pseudo-Goldstone bosons are approximately given by the Gell-Mann-Oakes-Renner relation

$$m_{PS}^2 = 2Bm_q\,, \tag{1}$$

where $B$ is a constant. In such a situation the point, where the pseudo-Goldstone bosons become massless, uniquely marks the vanishing of the quark masses.

QCD with one flavour of quarks ($N_f = 1$ QCD) radically differs from QCD with two or more flavours due to the absence of a chiral symmetry: there is no $\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R$ symmetry group, and the abelian $\mathrm{U}(1)_A$ symmetry of the one-flavour theory is washed out at the quantum level by the anomaly. As a consequence of this, the main features of the phase structure and mass spectrum of the single flavour theory strongly deviate from the familiar picture. In particular, there are no pseudo-Goldstone bosons, which would indicate the point of vanishing quark masses. In our project we undertake a thorough investigation of $N_f = 1$ QCD in order to study these fundamental questions.

A second interesting aspect is the possibility of a spontaneous breaking of CP (charge conjugation and parity) symmetry in QCD for special choices of the quark masses, conjectured for the first time by Dashen[3]. According to the Vafa-Witten theorem[4], a prerequisite for the spontaneous breaking of a discrete symmetry is a non-positive fermion measure, which in $N_f = 1$ QCD is possible for negative quark masses. The transition line is indeed expected to be located[5] on the negative real quark mass axis in the extended complex parameter space.

Another intriguing aspect of one-flavour QCD is the connection with the $\mathcal{N}$=1 supersymmetric Yang-Mills theory (SYM) in a particular limit of a large number of colours $N_c$[6]. An important place where relics of SUSY in $N_f = 1$ QCD can be investigated, is the low-lying bound-state spectrum[7]. Low-energy models for SYM[8] predict a low-lying chiral supermultiplet including two scalar particles with opposite parity. In $N_f = 1$ QCD these two particles can be identified with the $\eta$ and the $\sigma$ meson. Their mass ratio including $O(1/N_c)$ corrections is expected to be $m_\sigma/m_\eta = N_c/(N_c - 2)$[9].

## 2 Partially Quenched QCD

As we have argued in[7], it is useful to enhance the symmetry of the one-flavour theory by adding extra valence quarks which are *quenched*, i.e., not included in the fermion determinants. We take two valence quarks $u$ and $d$ with masses $m_V$ and one sea quark $s$ with mass $m_S$. For our purpose the case of degenerate valence and sea quark mass $m_V = m_S$ is particularly convenient. In this case the combined sea and valence sector is characterized by an exact $\mathrm{SU}(N_F)$ flavour symmetry, where $N_F \equiv N_V + N_f = 2 + 1$.

At the point of vanishing quark masses (see below) the generic partially quenched theory has a graded symmetry, which is broken spontaneously into a "flavour" symmetry $\mathrm{SU}(N_F|N_V)$, also valid for non-vanishing degenerate quark masses. The $\mathrm{SU}(N_F)$ subgroup represents the flavour symmetry in the combined sea and valence quark sectors. It implies that the hadronic bound states appear in exactly degenerate SU($N_F$) multiplets for $m_V = m_S$.

In particular, this extended theory contains a degenerate octet of pseudoscalar mesons ("pions" $\pi^a$, $a = 1, \ldots, 8$) satisfying an $\mathrm{SU}(3)$-symmetric PCAC relation. From the divergence of the axial-vector current and pseudoscalar density a bare *PCAC quark mass* can be naturally defined. Due to the exact SU(3)-symmetry, the corresponding renormalized quark mass $m^{\mathrm{R}}_{\mathrm{PCAC}}$ can be defined by an SU(3)-symmetric multiplicative renormalization.

As we will confirm numerically in Sec. 5, the masses of the "pions" can be made to vanish by suitably tuning the bare quark mass on the lattice. In this situation the renormalized quark mass vanishes, too. We stress here that the pions are not particles in the physical spectrum of the theory. Nevertheless, their properties as mass and decay constant are well defined quantities which can be computed on the lattice. The same applies for the PCAC quark mass, which can therefore be regarded as a potential candidate for a definition of the quark mass in this theory.

### 2.1 Chiral Perturbation Theory

We have calculated both the masses and decay constants of the pseudo-Goldstone bosons[7] in next-to-leading order of partially quenched chiral perturbation theory along the lines of Ref. 12, including $\mathcal{O}(a)$ lattice artifacts[11]. Leaving out the lattice corrections, the expressions for the renormalized pion masses and decay constants in terms of the (renormalized) PCAC quark mass are

$$
\begin{aligned}
m_\pi^2 &= \chi_{\mathrm{PCAC}} + \frac{\chi_{\mathrm{PCAC}}^2}{16\pi^2 F_0^2} \ln \frac{\chi_{\mathrm{PCAC}}}{\Lambda_3^2} \,, \\
\frac{f_\pi^{\mathrm{R}}}{F_0\sqrt{2}} &= 1 - \frac{\chi_{\mathrm{PCAC}}}{32\pi^2 F_0^2} \ln \frac{\chi_{\mathrm{PCAC}}}{\Lambda_4^2} \,,
\end{aligned}
\tag{2}
$$

where $\chi_{\mathrm{PCAC}} = 2B_0\, m^{\mathrm{R}}_{\mathrm{PCAC}}$ with the usual leading order low-energy constant $B_0$, and $\Lambda_3$ and $\Lambda_4$ are next-to-leading order low-energy constants.

The pion mass and the mass of the "physical" $\eta$ can be related by an extension of PQChPT[10,12]. The leading order expression for the mass of the $\eta$ reads

$$
m_\eta^2 = \frac{m_\Phi^2 + \chi_{\mathrm{PCAC}}}{1+\alpha}, \tag{3}
$$

where $\alpha$ and $m_\Phi$ are free parameters in this context. Our numerical results for $m_\eta$ allow to determine $\alpha$ and $m_\Phi$ (see Section 5).

## 3 Simulation

The present study[7] has been performed on a $12^3 \cdot 24$ lattice at inverse gauge coupling $\beta = 3.8$ and $16^3 \cdot 32$ lattice at $\beta = 4.0$. The lattice spacings correspond to $a \simeq 0.19\,\mathrm{fm}$ and $a \simeq 0.13\,\mathrm{fm}$, respectively. We use the Sommer parameter[13] $r_0$ for setting the scale, fixed at the conventional value $r_0 \equiv 0.5\,\mathrm{fm}$. The extensions of the lattices are roughly constant: $L = 2.23\,\mathrm{fm}$ and $L = 2.14\,\mathrm{fm}$.

For the fermions we use the Wilson action; in the SU(3) gauge sector we apply the tree-level improved Symanzik (tlSym) action[14]. The update algorithm is a Polynomial Hybrid

Monte Carlo algorithm (PHMC)[15,16] allowing the simulation of an odd number of fermion species. The present version[17] is based on a two-step polynomial approximation of the inverse fermion matrix with stochastic correction in the update chain, taken over from the two-step multi-boson algorithm of Ref. 18. We reached a relatively high total acceptance of 0.64–0.72. A correction factor in the measurement is associated with configurations for which eigenvalues of the (squared Hermitian) fermion matrix $Q^2[U]$ lie outside the validity interval of the polynomial approximation.

As indicated in the introduction, the sign of the quark determinant is an important issue in $N_f = 1$ QCD. With Wilson lattice fermions for small quark masses, it can become negative due to quantum fluctuations. The sign $\sigma[U]$ of the fermion determinant $\det Q[U]$ has to be included in the reweighting of the configurations. For its computation we applied two methods. In the first we studied the *spectral flow* of the Hermitian fermion matrix[19], following Ref. 20 for the computation of the low-lying eigenvalues. Alternatively, we computed the spectrum of the non-Hermitian matrix by ARPACK Arnoldi routines[21], concentrating on the lowest real eigenvalues: sign changes are signaled by negative real eigenvalues.

In most of our simulations the quark mass is large enough to prevent sign changes and the occurrence of a negative determinant is a rare event. On the other hand, for the smallest quark masses, $m_q \simeq 12\,\mathrm{MeV}$, a sizeable effect can be observed: the sign of the determinant pushes up the hadron masses by $7 - 10$%.

## 4 Hadron Spectrum

For the meson states we consider the simplest interpolating operators in the pseudoscalar and scalar sectors:

$$\eta(0^-): \quad P(x) = \bar{\psi}(x)\gamma_5\psi(x) \; , \tag{4}$$

$$\sigma(0^+): \quad S(x) = \bar{\psi}(x)\psi(x) \; . \tag{5}$$

Corresponding states in the QCD spectrum are the $\eta'(958)$ and $f_0(600)$ (or $\sigma$). The disconnected diagrams of the hadron correlators of $\eta$ and $\sigma$ were computed by applying stochastic sources with complex $Z_2$ noise and spin dilution[22].

In the baryon sector we considered a spin $3/2$ operator constructed from the quark field. The associated low lying state is expected to be the positive parity $(\frac{3}{2}^+)$ one. This corresponds to the $\Delta^{++}(1232)$ of QCD if our dynamical fermion is interpreted as a $u$ quark.

We used the single spatial plaquette to obtain the mass of the $0^{++}$ glueball state, employing APE smearing[23] and variational methods[24] to obtain optimal operators. Nevertheless, our statistics turned out not to be large enough to obtain an accurate estimate of the glueball masses.

The results for the hadron masses are plotted in Fig. 1 as a function of the bare PCAC quark mass. Since we use physical units here, results from the two lattice spacings can be compared. The scaling is satisfactory for the case of $\eta$, whose mass could be computed with the best accuracy. The determination of the $\sigma$ meson mass seems to require large statistics.

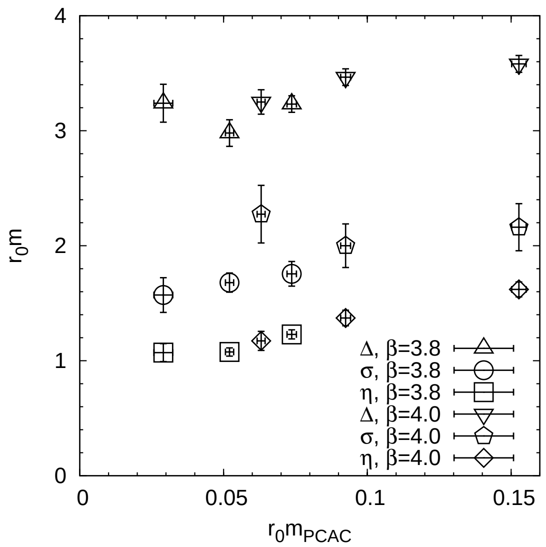


Figure 1. The mass of the lightest physical particles in one-flavour QCD as a function of the bare PCAC quark mass. The masses are multiplied by the scale parameter $r_0$ in order to obtain dimensionless quantities.

## 5 Partially Quenched Analysis

We have obtained results for the pion masses and decay constant and for the nucleon mass in the partially quenched sector. The partially quenched ChPT formulae are used to extract the corresponding low-energy coefficients from the pion data. Considering the number of lattice data at our disposal, a fit using the continuum terms and neglecting lattice artifacts is possible. We fitted the data for both $\beta$ values simultaneously neglecting the dependence of the renormalization factors $Z_A$ and $Z_P$ upon the lattice coupling constant. The data and the fitted curves are shown in Fig. 2. In order to improve the numerical results for the universal low-energy constants $\Lambda_{3,4}$, which do not explicitly depend on the lattice spacing $a$, we also performed fits to ratios of these quantities for the data at $\beta = 4.0$. We obtain in this case the results

$$\frac{\Lambda_3}{F_0} = 10.0 \pm 2.6\,, \tag{6}$$

$$\frac{\Lambda_4}{F_0} = 31.5 \pm 14.3\,, \tag{7}$$

which, interestingly, are compatible with phenomenological values obtained from ordinary QCD[25]. The errors are, however, quite large and we hope to improve these determinations in the future.

In addition, we investigated the relation between the mass of the pion and of the physical $\eta$ by fitting simultaneously $m_\pi^2$ and $m_\eta^2$ as a function of the PCAC quark mass according to formula (3), again considering only $\beta = 4.0$. Our data are consistent with a vanishing

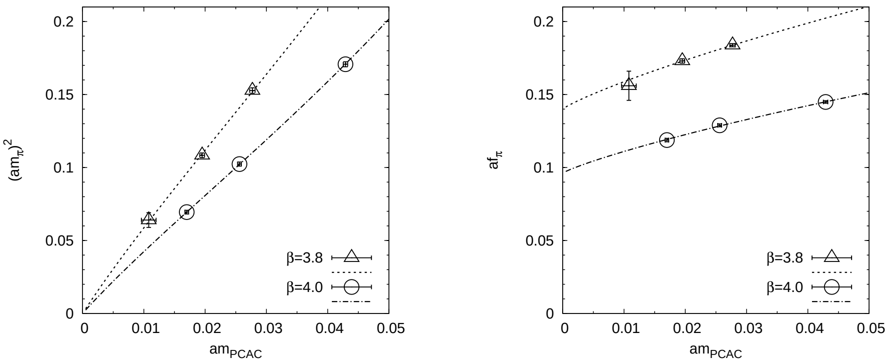


Figure 2. Pion masses squared and pion decay constants in lattice units and the results of the PQChPT fit.

$\alpha$. Setting $\alpha = 0$, we find

$$m_\Phi = 284 \pm 40\,\mathrm{MeV} \tag{8}$$

in physical units. The value of $m_\Phi$ can also be obtained from the Witten-Veneziano formula[26]

$$m_\Phi^2 = \frac{4N_f}{(f_\pi^{\mathrm{R}})^2}\chi_t \tag{9}$$

valid at leading-order in the ('t Hooft) large $N_c$ limit. An estimate of the quenched topological susceptibility[27] is $\chi_t = (193 \pm 9\,\mathrm{MeV})^4$. Using our value for $f_\pi^R$, which is subject to a sizeable statistical error, one would obtain $m_\Phi = 450 \pm 170\,\mathrm{MeV}$.

## 6 Summary and Outlook

This first Monte Carlo investigation of $N_f = 1$ QCD reveals the qualitative features of the low lying hadron spectrum of this theory. The lightest hadron is the pseudoscalar $\eta$ meson while the scalar meson, the $\sigma$, is about a factor 1.5 heavier. It is interesting to compare our data with the estimate in[28] $m_\sigma/m_\eta \simeq N_c/(N_c-2) = 3$ for $N_c = 3$. The above prediction applies for the massless theory and one could expect the agreement to improve for smaller quark masses. Our bare quark masses (estimated from the PCAC quark mass in the valence analysis) range between 10 MeV and 60 MeV, while the lightest pion mass is $\sim 270$ MeV.

The lightest baryon, the $\Delta$ $(\frac{3}{2}^+)$, is by about a factor 3 heavier than the $\eta$ meson. The lightest scalar mass obtained with a glueball $0^{++}$ operator lies between the $\sigma$ meson and the $\Delta$ baryon mass. However, this mass could be overestimated, since, due to the high level of noise, only small time-separations could be included in the analysis.

In general, the mass measurements have relatively large errors between 3–10%. In order to obtain more quantitative results, larger statistics and smaller quark masses are required. We hope to be able to make progresses in both directions[29] with our new simulations using Stout-smeared links in the fermion action. Some preliminary results have already been obtained.

The introduction of a partially quenched extension of the single flavour theory with valence quarks allows to define the bare quark mass in terms of the PCAC quark mass of the fictitious multi-flavour theory. Comparison of lattice data with partially quenched chiral perturbation theory allowed the determination of some of the low-energy constants of the chiral Lagrangian. The latter are compatible, even if with large error, with recent lattice determinations for $N_f = 2$ QCD.

A further direction of investigation for the future[29] is the CP-violating phase transition expected at negative quark masses[5]. For this aspect of the single flavour theory the non-positivity of the fermion measure plays an essential role.

## Acknowledgments

We are grateful to Luigi Scorzato for valuable discussions and help. We thank the John von Neumann Institute for Computing (NIC) and the computer center at DESY Hamburg for providing us the necessary technical help and computer resources. This work is supported in part by the Deutsche Forschungsgemeinschaft under grant Mu757/13-1. E.S. is supported by the U.S. Dept. of Energy under contract DE-AC02-98CH10886.

## References

1. M. Creutz, *Ambiguities in the up-quark mass*, Phys. Rev. Lett. **92**, 162003, 2004; hep-ph/0312225.
2. M. Creutz, *Spontaneous violation of CP symmetry in the strong interactions*, Phys. Rev. Lett. **92**, 201601, 2004; hep-lat/0312018.
3. R.F. Dashen, *Some features of chiral symmetry breaking*, Phys. Rev. D **3**, 1879, 1971.
4. C. Vafa and E. Witten, *Restrictions on symmetry breaking in vector-like gauge theories*, Nucl. Phys. B **234**, 173, 1984.
5. M. Creutz, *Quark masses and chiral symmetry*, Phys. Rev. D **52**, 2951, 1995; hep-th/9505112.
6. A. Armoni, M. Shifman and G. Veneziano, *Exact results in non-supersymmetric large N orientifold field theories*, Nucl. Phys. B **667**, 170, 2003; hep-th/0302163; A. Armoni and M. Shifman, *The cosmological constant and domain walls in orientifold field theories and N = 1 gluodynamics*, Nucl. Phys. B **670**, 148, 2003; hep-th/0303109; A. Armoni, M. Shifman and G. Veneziano, *SUSY relics in one-flavor QCD from a new 1/N expansion*, Phys. Rev. Lett. **91**, 191601, 2003; hep-th/0307097.
7. F. Farchioni, I. Montvay, G. Münster, E. E. Scholz, T. Sudmann and J. Wuilloud, *Hadron masses in QCD with one quark flavour*, Eur. Phys. J. C **52**, 305, 2007; arXiv:0706.1131 [hep-lat].
8. G. Veneziano and S. Yankielowicz, *An effective Lagrangian for the pure N=1 supersymmetric Yang-Mills theory*, Phys. Lett. B **113**, 231, 1982.
9. A. Armoni and E. Imeroni, *Predictions for orientifold field theories from type 0' string theory*, Phys. Lett. B **631**, 192, 2005; hep-th/0508107.
10. C. W. Bernard and M. F. L. Golterman, *Partially quenched gauge theories and an application to staggered fermions*, Phys. Rev. D **49**, 486, 1994; hep-lat/9306005.
11. G. Rupak and N. Shoresh, *Chiral perturbation theory for the Wilson lattice action*, Phys. Rev. D **66**, 054503, 2002; hep-lat/0201019.

12. S. R. Sharpe and N. Shoresh, *Partially quenched chiral perturbation theory without* $\Phi_0$, Phys. Rev. D **64**, 114510, 2001; hep-lat/0108003.
13. R. Sommer, *A new way to set the energy scale in lattice gauge theories and its applications to the static force and alpha-s in SU(2) Yang-Mills theory*, Nucl. Phys. B **411**, 839, 1994; hep-lat/9310022.
14. P. Weisz, *Continuum limit improved lattice action for pure Yang-Mills theory. 1*, Nucl. Phys. B **212**, 1, 1983; P. Weisz and R. Wohlert, *Continuum limit improved lattice action for pure Yang-Mills theory. 2,* Nucl. Phys. B **236**, 397, 1984 [Erratum-ibid. B **247**, 544, 1984].
15. P. de Forcrand and T. Takaishi, *Fast fermion Monte Carlo*, Nucl. Phys. Proc. Suppl. **53**, 968, 1997; hep-lat/9608093.
16. R. Frezzotti and K. Jansen, *A polynomial hybrid Monte Carlo algorithm*, Phys. Lett. B **402**, 328, 1997; hep-lat/9702016.
17. I. Montvay and E. Scholz, *Updating algorithms with multi-step stochastic correction*, Phys. Lett. B **623**, 73, 2005; hep-lat/0506006; E. E. Scholz and I. Montvay, *Multi-step stochastic correction in dynamical fermion updating algorithms*, PoS **LAT2006**, 037, 2006; hep-lat/0609042.
18. I. Montvay, *An algorithm for gluinos on the lattice*, Nucl. Phys. B **466**, 259, 1996; hep-lat/9510042.
19. R. G. Edwards, U. M. Heller and R. Narayanan, *Spectral flow, chiral condensate and topology in lattice QCD*, Nucl. Phys. B **535**, 403, 1998; hep-lat/9802016.
20. T. Kalkreuter and H. Simma, *An accelerated conjugate gradient algorithm to compute low lying eigenvalues: A study for the Dirac operator in SU(2) lattice QCD*, Comput. Phys. Commun. **93**, 33, 1996; hep-lat/9507023.
21. R. B. Lehoucq, D. C. Sorensen and C. Yang, 1997, `http://www.caam.rice.edu/software/ARPACK/`.
22. F. Farchioni and R. Peetz, *The low-lying mass spectrum of the N = 1 SU(2) SUSY Yang-Mills theory with Wilson fermions*, Eur. Phys. J. C **39**, 87, 2005; hep-lat/0407036.
23. M. Albanese *et al.* [APE Collaboration], *Glueball masses and string tension in lattice QCD*, Phys. Lett. B **192**, 163, 1987.
24. C. J. Morningstar and M. J. Peardon, *The glueball spectrum from an anisotropic lattice study*, Phys. Rev. D **60**, 034509, 1999; hep-lat/9901004.
25. J. Gasser and H. Leutwyler, *Chiral perturbation theory to one loop*, Annals Phys. **158**, 142, 1984; S. Dürr, *M(pi)**2 versus m(q): Comparing CP-PACS and UKQCD data to chiral perturbation theory*, Eur. Phys. J. C **29**, 383, 2003; hep-lat/0208051.
26. E. Witten, *Current algebra theorems for the U(1) Goldstone boson*, Nucl. Phys. B **156**, 269, 1979; G. Veneziano, *U(1) Without Instantons*, Nucl. Phys. B **159**, 213, 1979.
27. S. Dürr, Z. Fodor, C. Hoelbling and T. Kurth, *Precision study of the SU(3) topological susceptibility in the continuum*, JHEP **0704**, 055, 2007; hep-lat/0612021.
28. F. Sannino and M. Shifman, *Effective Lagrangians for orientifold theories*, Phys. Rev. D **69**, 125004, 2004; hep-th/0309252.
29. F. Farchioni, I. Montvay, G. Münster, E. E. Scholz, T. Sudmann and J. Wuilloud, in preparation.